Localised and nonlocalised structures in nonlinear lattices with fermions

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Abstract. – We discuss the quasiclassical approximation for the equations of motions of a nonlinear chain of phonons and electrons having phonon mediated hopping. Describing the phonons and electrons as even and odd grassmannian functions and using the continuum limit we show that the equations of motions lead to a Zakharov-like system for bosonic and fermionic fields. Localised and nonlocalised solutions are discussed using the Hirota bilinear formalism. Nonlocalised solutions turn out to appear naturally for any choice of wave parameters. The bosonic localised solution has a fermionic dressing while the fermionic one is an oscillatory localised field. They appear only if some constraints on the dispersion are imposed. In this case the density of fermions is a strongly localised travelling wave. Also it is shown that in the multiple scales approach the emergent equation is *linear*. Only for the resonant case we get a nonlinear fermionic Yajima-Oikawa system. Physical implications are discussed.

Introduction. – The idea of treating classically systems with fermions goes back to seventies to the papers of Berezin [1], Casalbuoni [2]. This is done using grassmannian functions (elements of a Grassmann algebra). A simple representation can be done using, for instance, combinations of Dirac matrices, namely $\alpha = \gamma_1 + i\gamma_2, \beta = \gamma_3 + i\gamma_4$. The algebra generated by $(1, \alpha, \beta, \alpha\beta)$ is a grassmann algebra with two generators. The even sector (bosonic or commutative) is given by linear combinations of $(1, \alpha\beta)$, while the odd sector (fermionic or anticommutative) is given by linear combinations of (α, β).

Today, grassmannian description is used intensively in mathematical physics. It is a very interesting idea because it could be implemented to nonlinear evolution equations containing bosons and fermions, for which the quantum description is difficult to do. Moreover, since the quantum mechanics deals mainly with observables and spectra, classical description offers an idea of the dynamics of solutions for the equations of motions. In this view there are some results related to the dynamics of solitons in integrable equations containing bosons and fermions but linked supersymmetrically [3]. With the aid of a supersymmetric bilinear formalism these type of equations have been solved. Interesting enough the existence of fermions makes the soliton interaction to be nonelastic having a dressing in the fermionic part.

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Due to these new results it seems naturally to try to extend them to some physical models involving bosons and fermions and to see how the dynamics of the localised solutions is influenced by the fermions.

The main realm is of course the problem of localised structures in biomolecules (proteins, DNA, etc.). Since the seminal ideas of A. S. Davydov [4], it has been continuing an intense quest for finding experimentally these nonlinear structures (solitons, breathers, etc.) [5]. In any case, insofar the results are controversial.

In this paper we consider the simplest model namely a nonlinear chain and describe the phonons and electrons as functions having values in the even and the odd sector of an infinitely generated grassmann algebra (this can be done either directly or using coherent states). The choice of SSH hamiltonian is not only for simplicity, but also it captures the essential informations when one deals with a nonlinear lattice having a coupling between charge and structure (which explains charge conduction, polaron formation etc.) [6], [7].

In the continuum limit the differential-difference equations of motions become a system which looks like the classical Zakharov system [8] with fermions. Interesting enough this system admits exact bilinearisation in the Hirota formalism and *two* type of solutions. One type is exponential and nonlocalised although it appears to look like a kink type solution. But the presence of fermionic parameters at denominators breaks the localisation. The other type is localised even though is dressed with fermionic parameters as well. This type of solutions is responsible for a soliton-like propagating structure of the fermionic density in the chain.

Equations of motion. – The hamiltonian we are working with is

$$\mathcal{H} = \sum_n \frac{\dot{u}_n^2}{2} + W(u_{n+1} - u_n) + (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1})\,[-t_0 + \gamma(u_{n+1} - u_n)] \qquad (1)$$

where u_n is the displacement from the equilibrium position of the particle n and $c_n^\dagger(c_n)$ are the creation (annihilation) operators for fermions on the site n. Also the potential $W(u_{n+1} - u_n)$ can be harmonic as in the Su-Schriffer-Heeger (SSH) problem [6] or anharmonic. We do not consider the spin indices because we are not interested here in magnetic phenomena. The last term which contains the phonon mediated hopping is responsible for the interesting physics of the system. The classical hamiltonian can be obtained by averaging the quantum one using the product of the following coherent states (or directly by substitution)

$$|\chi_n >= e^{-\chi_n^*\chi_n/2} e^{\chi_n c_n^\dagger}|0>,$$

where $\chi_n(t)$ are grassmann-valued odd (anticommuting) complex functions. Also $u_n(t)$ are, from now on grassmann-valued even (commuting) functions (they are *not* real functions anymore). They belong to the even and odd sector of an infinitely generated grassmann algebra. Complex conjugation is defined such that $(z_1 z_2)^* = z_2^* z_1^*$ in accordance with the conventions in [9]. As we are dealing with the classical case we assume further that all fields and their derivatives commute or anticommute, depending in the usual way on the bosonic or fermionic nature of the fields.

First we consider the harmonic approximation, namely $W(u_{n+1} - u_n) = K/2(u_{n+1} - u_n)^2$. After averaging on the coherent states we find the following classical hamiltonian.

$$H = \sum_n \frac{\dot{u}_n^2}{2} + \frac{K}{2}(u_{n+1} - u_n)^2 + (\chi_{n+1}^*\chi_n + \chi_n^*\chi_{n+1})\,[-t_0 + \gamma(u_{n+1} - u_n)] \qquad (2)$$

The equations of motions are given by [2]:

$$\ddot{u}_n = K(u_{n+1} + u_{n-1} - 2u_n) + \gamma(\chi_{n+1}^*\chi_n + \chi_n^*\chi_{n+1} - \chi_n^*\chi_{n-1} - \chi_{n-1}^*\chi_n) \qquad (3)$$

$$i\dot{\chi}_n = -t_0(\chi_{n+1} + \chi_{n-1}) + \gamma\left[(u_n - u_{n-1})\chi_{n-1} + (u_{n+1} - u_n)\chi_{n+1}\right] \tag{4}$$

A tractable version of the above equations can be obtained using their continuum limit. Considering $x = \epsilon n$ we keep only terms up to order two in the expansions, i.e. $u_{n\pm1} = u(x,t) \pm u_x + u_{xx}/2$ and the same for $\chi_{n\pm1}$. After gauging the fermionic field $\chi \to \chi \exp(-2it_0 t)$ and calling $K = c^2$ we find the following system:

$$u_{tt} - c^2 u_{xx} = 2\gamma(\chi^*\chi)_x \tag{5}$$

$$i\chi_t + t_0\chi_{xx} - 2\gamma u_x \chi = 0 \tag{6}$$

As expected we get the Zakharov system with bosonic and fermionic components. The corresponding hamiltonian for these equations is given by:

$$H = \int dx \left(\frac{1}{2}u_t^2 + \frac{c^2}{2}u_x^2 + 2\gamma\chi^*\chi u_x + t_0\chi_x^*\chi_x\right) \tag{7}$$

Localised and nonlocalised solutions. – In order to solve the equations of motions (5), (6) one can write all the quantities in terms of the generators of Grassmann algebra and then solve the equations layer by layer [10]. Even though the results can be very interesting, they depend on the number of generators. A different approach which is more appropriate for computing the soliton-like solutions is the Hirota bilinear method [11]. The idea behind it is to implement a nonlinear substitution for the field such that the nonlinear system is turned into a bilinear one having the form of the dispersion relation when is written using the Hirota operators. On the other hand the nonlinear substitution somehow swallows the singularities of the solutions of nonlinear system and the bilinear one become a system which contains holomorphic functions. In the case of integrable systems this fact is rigurously true. But in the case of nonintegrable systems this works only for special solutions which, because of the holomorphic character, can be written in terms of exponentials. This strongly alleviates all the calculations. On the other hand the adaptation of Hirota formalism to grassmannian functions is straightforward.

The nonlinear substitutions are:

$$\chi(x,t) = \frac{\sqrt{t_0}}{2\gamma}\frac{G}{F}, \quad u(x,t) = -\frac{t_0}{\gamma}\partial_x \log F$$

where $G(x,t)$ is an grassmann anticommuting complex function and F is a grassmann commuting real function. Plugging into the nonlinear equations we find the following bilinear system:

$$(\mathbf{D}_t^2 - c^2\mathbf{D}_x^2)F \bullet F = GG^* \tag{8}$$

$$(i\mathbf{D}_t + t_0\mathbf{D}_x^2)G \bullet F = 0 \tag{9}$$

where $\mathbf{D}_x^n f \bullet g = (\partial_\epsilon)^n f(x+\epsilon)g(x-\epsilon)|_{\epsilon=0}$ is the Hirota bilinear operator. Now, usually the second bilinear equation gives the dispersion relation and the other one is only a constraint on the phases. The 1-soliton solution usually is given by the following ansatz,

$$G = \zeta e^{\eta}, \quad F = 1 + e^{\eta+\eta^*+\phi} \tag{10}$$

where ζ is a complex anticommuting grassmann parameter ($\zeta = \zeta_R + i\zeta_I$), $\eta = kx + \omega t$ where k and ω are commuting complex grassmann parameters and ϕ a constant phase. After plugging the ansatz into the equation we find the following relations for the parameters:

$$\left[(\omega+\omega^*)^2 - c^2(k+k^*)^2\right]e^{\phi} = \frac{1}{2}\zeta\zeta^* \tag{11}$$

$$i\omega + t_0 k^2 = \alpha\zeta\zeta^* \tag{12}$$

The second equation and its complex conjugate arise as overall factors multiplicating terms containing ζ and ζ^*. Accordingly these factors must be zero or proportional with the product $\zeta\zeta^*$ by a complex factor α.

Case $\alpha = 0$

As we pointed out, the eq. (12) gives the dispersion relation of the soliton and the equation (11) is necessary to compute the phase ϕ. Indeed, in our case,

$$e^{\phi} = \frac{\zeta\zeta^*}{2(\omega+\omega^*)^2 - 2c^2(k+k^*)^2}$$

i.e. is proportionally with the product of zetas. So, there are absolutely no restrictions on k and ζ. For simplicity let's call the denominator denominator Λ^{-1}. Our 1-soliton solution will be (up to the factors)

$$\chi(x,t) = \frac{G}{F} = \frac{\zeta e^{\eta}}{1+\Lambda\zeta\zeta^* e^{\eta+\eta^*}}, \quad u(x,t) = \frac{F_x}{F} = \frac{(k+k^*)\Lambda\zeta\zeta^* e^{\eta+\eta*}}{1+\Lambda\zeta\zeta^* e^{\eta+\eta^*}}$$

In the grassmann algebra we can compute exactly the inverse of an commuting object, namely $1/(a+b\zeta_1\zeta_2) = 1/a - \zeta_1\zeta_2 b/a^2$ and this is because of the fact that $\zeta_i^2 = 0$. Applying this rule to our soliton we shall find that our soliton is not at all a soliton but a pure **nonlocalised** exponential solution.

$$\chi(x,t) = \zeta e^{\eta}, \quad u(x,t) = (k+k^*)\Lambda\zeta\zeta^* e^{\eta+\eta^*} \tag{13}$$

One can see that the bosonic solution is purely grassmannian (its square is zero), so we can speculate that it exists only at the quantum level. Accordingly, the usual method of finding localised solutions for Hirota bilinear equations here fails due to the grassmannian character of the parameters.

There is a big drawback of these solutions. They have no physical meaning since they grow exponentially and the energy as well.

So we are forced to look for a method to find localised solutions. A posibility is to treat diferently equation (11), namely to take it *as a dispersion relation* while the equation (12) will give *constraints* on the solitonic parameters. For instance we can consider that e^{ϕ} is not at all proportional to the product of zetas but just a pure number (let's say 1/8) and zeta's enter in a the relation of ω and k i.e

$$(\omega+\omega^*)^2 - c^2(k+k^*)^2 = e^{-\phi}\zeta\zeta^*/2$$

If we put $\omega = \omega_R + i\omega_I$, $k = k_R + ik_I$ and $e^{\phi} = 1/8$ we find the following relation

$$\omega_R = \sqrt{c^2k_R^2 + \zeta\zeta^*} = ck_R + \frac{1}{2ck_R}\zeta\zeta^* = ck_R + \frac{i}{ck_R}\zeta_I\zeta_R$$

the last equations being consequences of the grassmannian character of ζ and ζ^*. Also the last equation is a *real* grassmannian quantity despite the i factor because of the definition of complex conjugation $(z_1z_2)^* = z_2^*z_1^*$. Plugging this relation into the equation (12) one obtains

$$k_I = -\left(\frac{c}{2t_0} + \frac{\zeta\zeta^*}{4t_0k_R^2c}\right), \quad \omega_I = t_0\left(k_R^2 - \frac{c^2}{4t_0^2} - \frac{\zeta\zeta^*}{4t_0^2k_R^2}\right)$$

These are the constraints in the sense that k_I and ω_I are no longer free. So, instead of having four free parameters k_R, k_I, ζ_R, ζ_I we have only three k_R, ζ_R and ζ_I. With all these relations one can write (after some algebra) completely the 1-soliton solution,

$$u(x,t) = \frac{k_R}{2} sech^2 \eta_0 \left(e^{2\eta_0} + \frac{1}{k_R c} e^{t\zeta\zeta^*} \right) \tag{14}$$

$$\chi(x,t) = \frac{\zeta}{2} sech \eta_0 \exp \left[-i \frac{c}{2t_0} x - i(k_R^2 t_0 - \frac{c^2}{4t_0}) t \right] \tag{15}$$

where $\eta_0 = k_R x + c k_R t$. One can see that the fermionic field χ is indeed a localised field with an oscillating amplitude. The problem of localisability for the bosonic field is not so obvious because of the fermionic *dressing* in the last exponential. In any case expanding the exponential (taking into account that the square of $\zeta\zeta^*$ is zero) we see that the problematic part of $u(x,t)$ is $(t/k_R c) sech^2 \eta_0$ which *has* finite limits as time goes to infinity. So we have indeed a **localised solution** which is expressed using bosonic and fermionic parameters. The bosonic field contain a fermionic correction and the fermionic field is a soliton with oscillating complex amplitude. Here the physical interpretation is clear. This can be seen as a classical analog of the localised polaron wave function for the SSH problem [7]. With our method we can in principle prove the existence of localised states. Using this solution one can compute the behaviour of the fermionic density, namely $c_n^\dagger c_n$. In the continuum limit this expression is given by

$$\chi^*(x,t)\chi(x,t) = \frac{\zeta^*\zeta}{4} sech^2 \eta_0$$

which shows the strongly localised character of the charge density travelling wave. Plugging these solutions in the expression of the hamiltonian (7) we find the energy:

$$H = \frac{2k_R t_0^2 c^2}{3\gamma^2} + \frac{2t_0^2}{3\gamma^2} \left(2k_R + \frac{1}{k_R} \right) \zeta\zeta^*$$

One can see that the dressing of the bosonic solution and the fermionic field gives a purely grassmannian correction.

Case $\alpha \neq 0$

In this case, considering $\alpha = \mu + i\nu$ the relations for k_I and ω_I have the same structure. Only the factors of zetas are translated with some terms proportional with μ and ν.

Of course, a big advantage of this model is that the underlying bosonic part is just a linear Klein-Gordon equation, so we do not have solitonic phenomenology. We can do absolutely the same machinery for a nonlinear completely integrable bosonic equation with rich solitonic phenomenology. For instance, we consider a fermionic extension of the Boussinesq equation

$$u_{tt} - u_{xx} - 6u_x u_{xx} - u_{xxxx} = (\chi\chi^*)_x \tag{16}$$

$$i\chi_t + \chi_{xx} - 2u_x \chi = 0 \tag{17}$$

This system can be seen as a continuum version of the equations of motions for the hamiltonian (2.1) with the potential (up to coefficients) $W(u_{n+1} - u_n) = 1/2(u_{n+1} - u_n)^2 + 1/3(u_{n+1} - u_n)^3$ for a weak phonon mediated hopping (we neglected the coefficients in the equations). Then with the same nonlinear substitution we shall get:

$$(\mathbf{D}_t^2 - \mathbf{D}_x^2 - \mathbf{D}_x^4) F \bullet F = G^* G, \quad (i\mathbf{D}_t + \mathbf{D}_x^2) G \bullet F = 0 \tag{18}$$

The ansatz for 1-soliton solution gives the following dispersion relations

$$\left[(\omega+\omega^*)^2-(k+k^*)^2-(k+k^*)^4\right]e^{\phi}=\frac{1}{2}\zeta^*\zeta,\quad i\omega+k^2=\alpha\zeta^*\zeta \tag{19}$$

One can see that everything works in the same way except that Λ^{-1} is translated with $(k+k^*)^4$.

Multiple scales approach. – Even though the continuum limit used above is a *naive* one we can prove that using the systematic multiple scales method [12] one gets the unidirectional approximation of the system (2.5), (2.6).

In order to do this we assume that the competition between dispersion and nonlinearity occurs at large scales of space and time. Accordingly, we introduce the following stretched variables:

$$\xi=\epsilon(n-v_g t),\quad \tau=\epsilon^2 t$$

and consider that the fermionic complex field is just a slowly modulated fermionic wave,

$$\chi_n(t)=e^{i(kn-\omega t)}\sum_{j\ge 1}\epsilon^j\Phi_j(\xi,\tau).$$

In the exponential, ω is exactly the dispersion relation of the *second* discrete equation from the system (3), namely $\omega=-2t_0\cos k$. Also v_g in the definition of the streched space is the group velocity corresponding to this dispersion. For the bosonic field we take,

$$u_n(t)=\sum_{j\ge 1}\epsilon^j W_j(\xi,\tau)$$

Using the discrete equations (4) we shall find at the order ϵ^3

$$i\Phi_{1\tau}=-\omega_2\Phi_{1\xi\xi}-2\gamma\cos k W_{1\xi}\Phi_1$$

where $\omega_2=d^2\omega/dk^2$. Also from the first discrete equation (3) we shall find

$$\epsilon^3(v_g^2-c^2)W_{1\xi\xi}+\mathcal{O}(\epsilon^4)=2\gamma\epsilon^3\cos k(\Phi_1^*\Phi_1)_\xi+\mathcal{O}(\epsilon^4) \tag{20}$$

where c^2 is the phononic velocity. Assuming that we have the nonresonant case namely $v_g\neq c$ we find

$$W_{1\xi}=\frac{2\gamma\cos k}{v_g^2-c^2}\Phi_1^*\Phi_1$$

Introducing this in the above equation and taking into account that the square of the Φ_1 is zero we get a **linear** equation

$$i\Phi_{1\tau}+\omega_2\Phi_{1\xi\xi}=0 \tag{21}$$

Accordingly, in the nonresonant case there is no localised solution.

For the resonant case i.e. $v_g=c$ we have to change the scaling of the fermion field

$$\chi_n(t)=e^{i(kn-\omega t)}\sum_{j\ge 1}\epsilon^{j+1/2}\Phi_j(\xi,\tau)$$

which leaves unchanged the second equation but the first one will be

$$\epsilon^3(v_g^2-c^2)W_{2\xi\xi}-2\epsilon^4 v_g W_{1\xi\tau}+\mathcal{O}(\epsilon^5)=2\epsilon^4\gamma\cos k(\Phi_1^*\Phi_1)_\xi+\mathcal{O}(\epsilon^5)$$

Because $v_g = c$, finally we have the following system:

$$W_{1\tau} + \frac{\gamma}{v_g} \cos k (\Phi_1^* \Phi_1) = 0 \tag{22}$$

$$i\Phi_{1\tau} + \omega_2 \Phi_{1\xi\xi} + 2\gamma \cos k W_{1\xi} \Phi_1 = 0 \tag{23}$$

which is indeed the uni-directional approximation of the Zakharov-type system, the so called Yajima-Oikawa system [13]. This equation has also a bilinear form and we can compute the solutions in exactly the same way.

Conclusions. – The dynamics of localised solutions in a nonlinear chain with fermions described by SSH model. is solved here using bilinear formalism adapted to a grassmannian formulation of the equations of motions. The main problem here was that the usual way of finding solitonic solutions gives purely exponential nonlocalised solutions. This fact happens even in the case of supersymmetric integrable equations [14] using the celebrated Darboux transform. Anyway including the grassmannian parameters into the dispersion relation we have found really localised solutions but with some constraints on the parameters. So, one can speculate that in the nonlinear equations with fermions localised solutions exist only in special cases.

Also from the above multiple scale approach we can see that the existence of localised solutions is somehow problematic at least for SSH model inasmuch the general nonresonant case in the standard scaling goes to a linear equation for the fermionic field. Of course one can argue that a totally different scaling of space, time and fields might give a nonlinear equation for the fermionic field. We do not believe this since purely fermions cannot selforganize into solitons due to the exclusion principle. In order to appear localised solutions into a fermionic equation this one must be coupled with a bosonic one.

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